



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XDL
Title : Structure of human aldolase B associated with hereditary fructose intolerance (A149P), at 277K
Authors : Malay, A.D.; Allen, K.N.; Tolan, D.R.
Deposited on : 2004-09-07
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

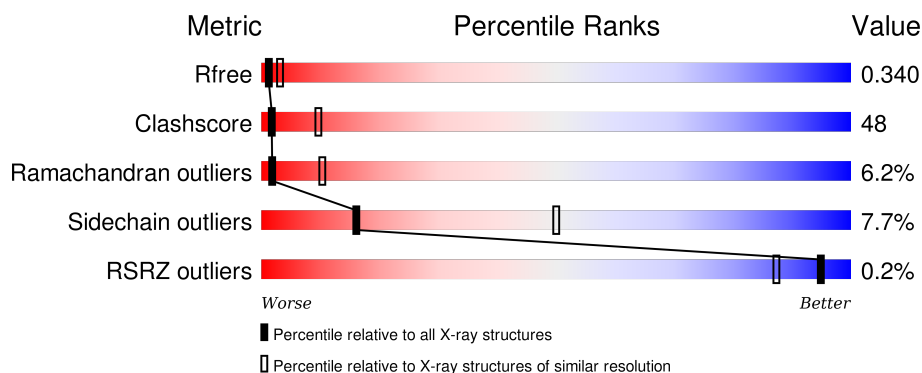
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div>31%</div> <div>45%</div> <div>7%</div> <div>17%</div> </div>
1	B	365	<div> <div>27%</div> <div>47%</div> <div>8%</div> <div>18%</div> </div>
1	C	365	<div> <div>29%</div> <div>52%</div> <div>8%</div> <div>10%</div> </div>
1	D	365	<div> <div>30%</div> <div>44%</div> <div>7%</div> <div>19%</div> </div>
1	W	365	<div> <div>29%</div> <div>45%</div> <div>6%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	X	365	<div><div></div><div>31%49%9%10%</div></div>
1	Y	365	<div><div></div><div>26%49%7%17%</div></div>
1	Z	365	<div><div>%</div><div></div><div>29%46%7%18%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18932 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fructose-bisphosphate aldolase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2331	1469	411	439	12			
1	B	299	Total	C	N	O	S	0	0	0
			2298	1448	405	433	12			
1	C	329	Total	C	N	O	S	0	0	0
			2527	1589	446	479	13			
1	D	297	Total	C	N	O	S	0	0	0
			2282	1436	403	431	12			
1	W	296	Total	C	N	O	S	0	0	0
			2274	1431	400	431	12			
1	X	329	Total	C	N	O	S	0	0	0
			2523	1584	445	481	13			
1	Y	302	Total	C	N	O	S	0	0	0
			2318	1460	408	438	12			
1	Z	301	Total	C	N	O	S	0	0	0
			2318	1461	408	437	12			

There are 24 discrepancies between the modelled and reference sequences:

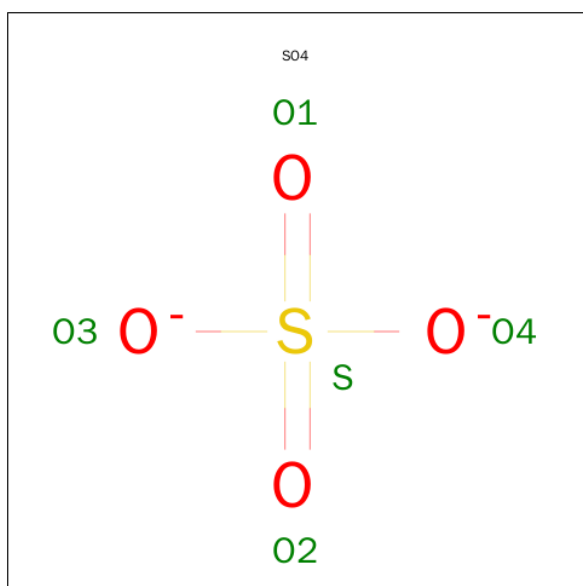
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P05062
A	0	SER	-	CLONING ARTIFACT	UNP P05062
A	149	PRO	ALA	ENGINEERED	UNP P05062
B	-1	GLY	-	CLONING ARTIFACT	UNP P05062
B	0	SER	-	CLONING ARTIFACT	UNP P05062
B	149	PRO	ALA	ENGINEERED	UNP P05062
C	-1	GLY	-	CLONING ARTIFACT	UNP P05062
C	0	SER	-	CLONING ARTIFACT	UNP P05062
C	149	PRO	ALA	ENGINEERED	UNP P05062
D	-1	GLY	-	CLONING ARTIFACT	UNP P05062
D	0	SER	-	CLONING ARTIFACT	UNP P05062
D	149	PRO	ALA	ENGINEERED	UNP P05062
W	-1	GLY	-	CLONING ARTIFACT	UNP P05062

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Chain	Residue	Modelled	Actual	Comment	Reference
W	0	SER	-	CLONING ARTIFACT	UNP P05062
W	149	PRO	ALA	ENGINEERED	UNP P05062
X	-1	GLY	-	CLONING ARTIFACT	UNP P05062
X	0	SER	-	CLONING ARTIFACT	UNP P05062
X	149	PRO	ALA	ENGINEERED	UNP P05062
Y	-1	GLY	-	CLONING ARTIFACT	UNP P05062
Y	0	SER	-	CLONING ARTIFACT	UNP P05062
Y	149	PRO	ALA	ENGINEERED	UNP P05062
Z	-1	GLY	-	CLONING ARTIFACT	UNP P05062
Z	0	SER	-	CLONING ARTIFACT	UNP P05062
Z	149	PRO	ALA	ENGINEERED	UNP P05062

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	W	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	X	1	Total O S 5 4 1	0	0
2	Y	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

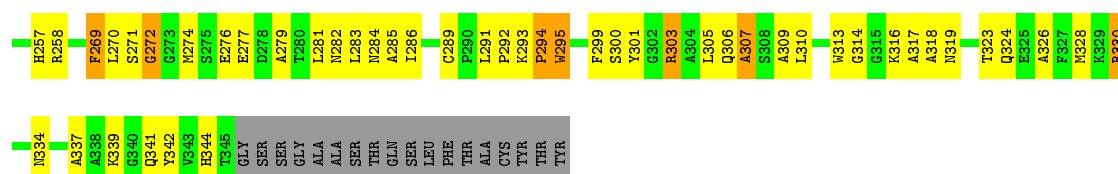
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	Y	1	Total	O	S	0	0
			5	4	1		

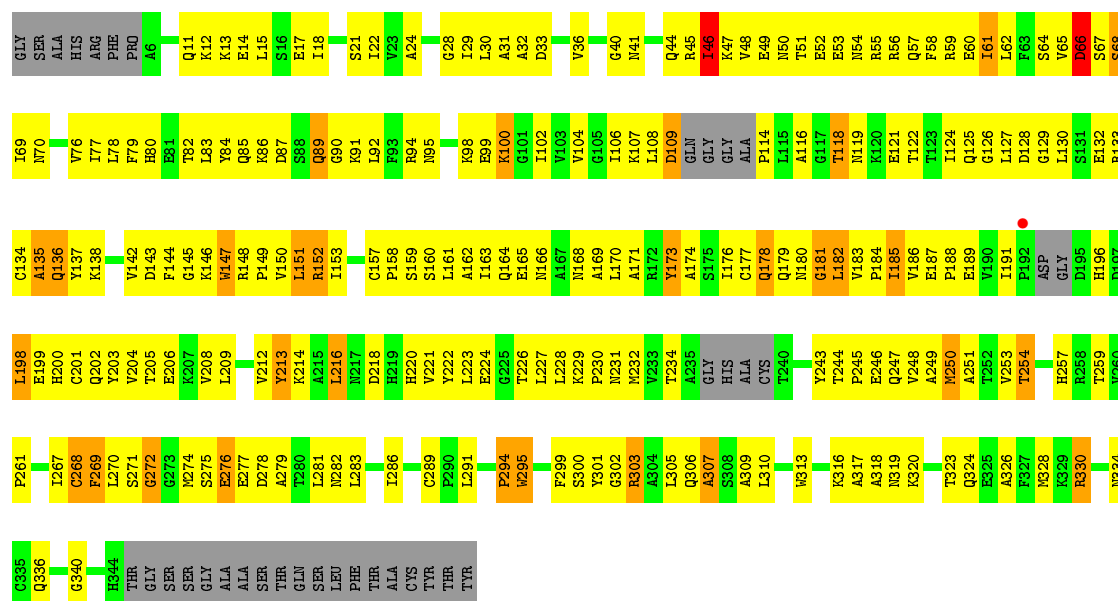
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	4	Total	O	0	0
			4	4		
3	C	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		
3	W	2	Total	O	0	0
			2	2		
3	X	1	Total	O	0	0
			1	1		
3	Y	2	Total	O	0	0
			2	2		
3	Z	3	Total	O	0	0
			3	3		



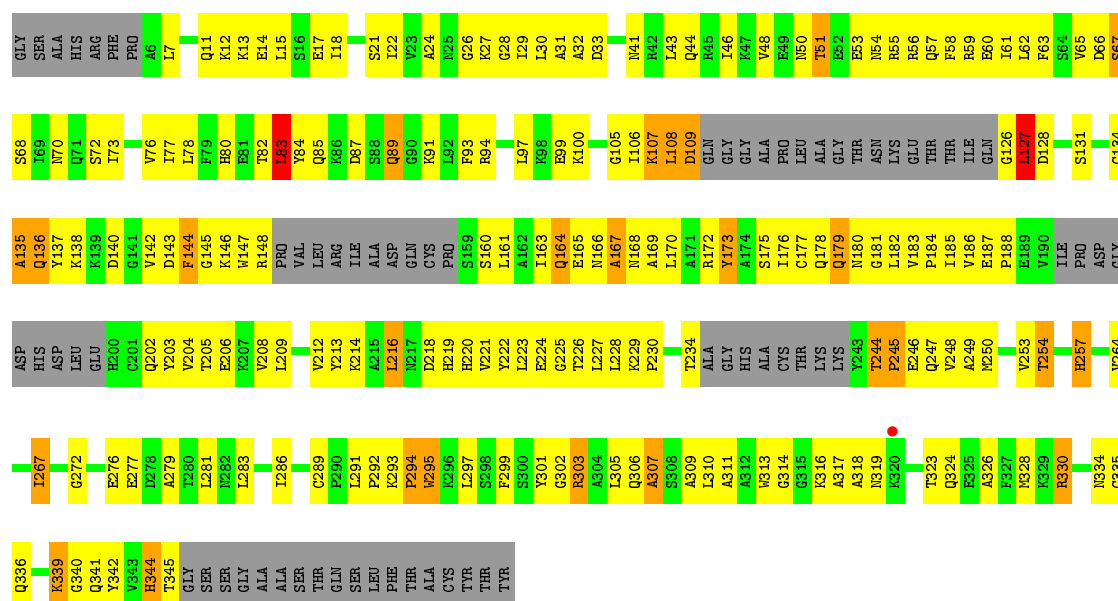
• Molecule 1: Fructose-bisphosphate aldolase B

Chain C: 29% 52% 8% 10%

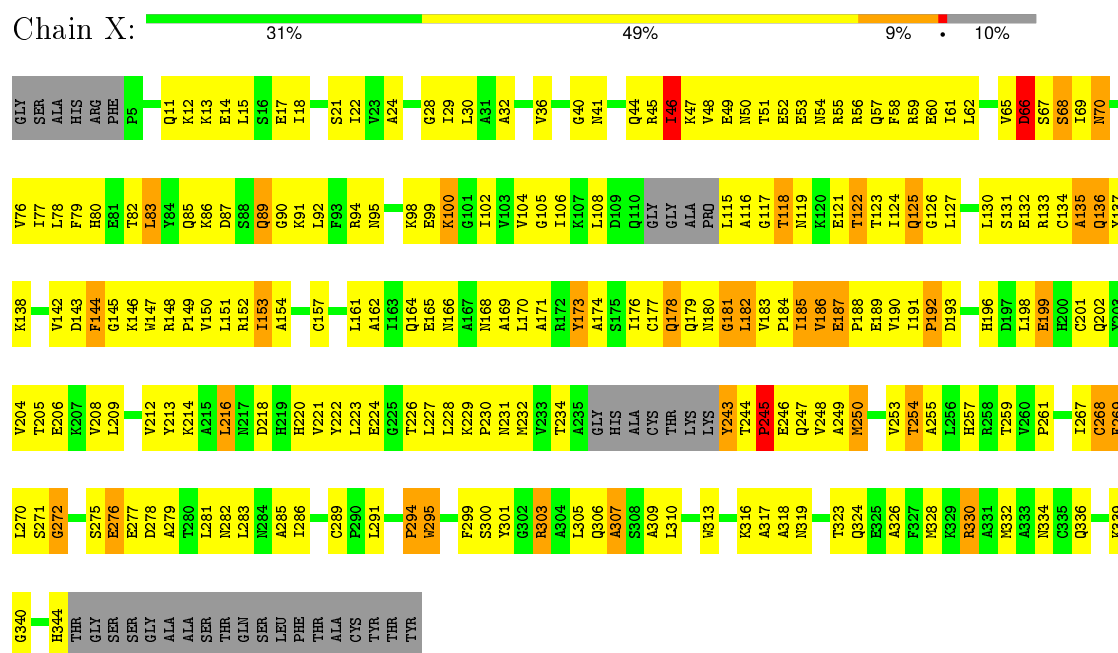
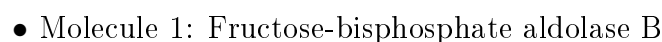


• Molecule 1: Fructose-bisphosphate aldolase B

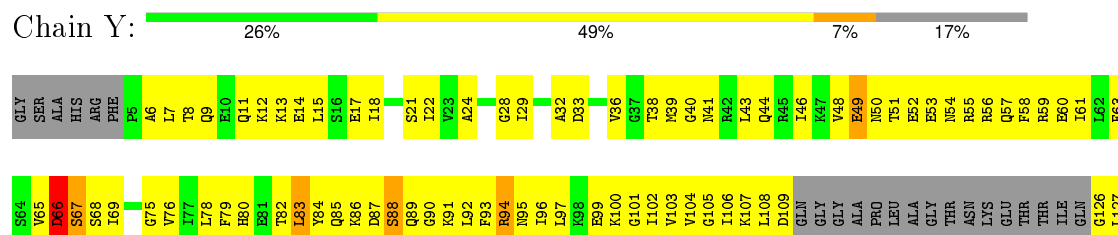
Chain D: 30% 44% 7% 19%

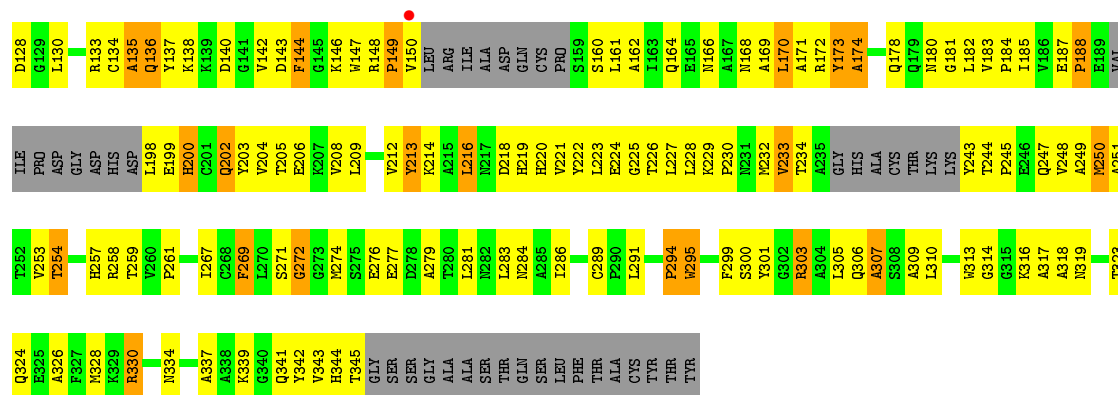


• Molecule 1: Fructose-bisphosphate aldolase B

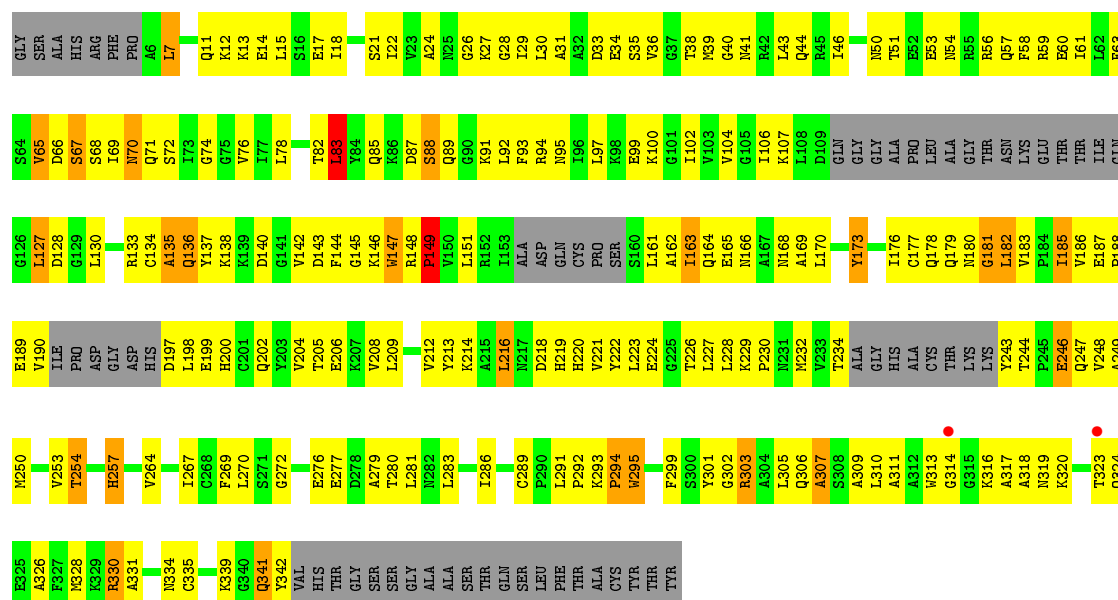


- Molecule 1: Fructose-bisphosphate aldolase B





• Molecule 1: Fructose-bisphosphate aldolase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.48Å 153.51Å 186.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.15 – 3.00 20.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.1 (20.15-3.00) 69.9 (20.15-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.304 , 0.349 0.299 , 0.340	Depositor DCC
R_{free} test set	7001 reflections (10.13%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.8	EDS
Estimated twinning fraction	0.458 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 134381 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18932	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2365	0.67	0/3190
1	B	0.48	0/2333	0.71	0/3146
1	C	0.48	0/2566	0.72	1/3465 (0.0%)
1	D	0.42	0/2315	0.69	0/3121
1	W	0.42	0/2306	0.67	0/3108
1	X	0.48	1/2563 (0.0%)	0.74	2/3464 (0.1%)
1	Y	0.46	0/2353	0.71	0/3174
1	Z	0.40	0/2351	0.66	0/3170
All	All	0.44	1/19152 (0.0%)	0.70	3/25838 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	W	0	1
1	Y	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	70	ASN	CB-CG	-5.20	1.39	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	70	ASN	CB-CA-C	-10.72	88.96	110.40
1	X	66	ASP	N-CA-C	5.65	126.26	111.00
1	C	66	ASP	N-CA-C	5.43	125.65	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	TYR	Sidechain
1	C	213	TYR	Sidechain
1	C	84	TYR	Sidechain
1	W	213	TYR	Sidechain
1	Y	213	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2331	0	2359	214	0
1	B	2298	0	2313	247	0
1	C	2527	0	2555	262	0
1	D	2282	0	2301	220	0
1	W	2274	0	2293	201	0
1	X	2523	0	2538	259	0
1	Y	2318	0	2338	242	0
1	Z	2318	0	2345	220	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
2	Y	10	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	2	0
3	D	2	0	0	0	0
3	W	2	0	0	0	0
3	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Y	2	0	0	0	0
3	Z	3	0	0	1	0
All	All	18932	0	19042	1839	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 1839 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:303:ARG:H	1:W:303:ARG:HD2	1.05	1.19
1:Z:228:LEU:HG	1:Z:230:PRO:HD3	1.26	1.17
1:B:303:ARG:H	1:B:303:ARG:HD2	1.02	1.17
1:C:303:ARG:HD2	1:C:303:ARG:H	1.03	1.17
1:C:149:PRO:HG3	1:C:170:LEU:HD11	1.20	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/365 (80%)	223 (76%)	55 (19%)	15 (5%)	2	15
1	B	289/365 (79%)	209 (72%)	59 (20%)	21 (7%)	1	6
1	C	321/365 (88%)	244 (76%)	57 (18%)	20 (6%)	2	10
1	D	287/365 (79%)	218 (76%)	51 (18%)	18 (6%)	2	9
1	W	286/365 (78%)	222 (78%)	47 (16%)	17 (6%)	2	11
1	X	323/365 (88%)	246 (76%)	56 (17%)	21 (6%)	1	8
1	Y	292/365 (80%)	214 (73%)	60 (20%)	18 (6%)	2	10
1	Z	291/365 (80%)	219 (75%)	55 (19%)	17 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2382/2920 (82%)	1795 (75%)	440 (18%)	147 (6%)	2	10

5 of 147 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	149	PRO
1	A	233	VAL
1	B	67	SER
1	B	88	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/292 (85%)	230 (93%)	17 (7%)	19	56
1	B	242/292 (83%)	225 (93%)	17 (7%)	19	55
1	C	269/292 (92%)	247 (92%)	22 (8%)	14	46
1	D	241/292 (82%)	220 (91%)	21 (9%)	13	43
1	W	240/292 (82%)	223 (93%)	17 (7%)	18	54
1	X	268/292 (92%)	243 (91%)	25 (9%)	11	39
1	Y	245/292 (84%)	227 (93%)	18 (7%)	17	52
1	Z	245/292 (84%)	229 (94%)	16 (6%)	21	58
All	All	1997/2336 (86%)	1844 (92%)	153 (8%)	16	50

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	244	THR
1	W	173	TYR
1	Z	147	TRP
1	D	257	HIS
1	W	51	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	GLN
1	W	166	ASN
1	Z	95	ASN
1	D	219	HIS
1	W	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	364	-	4,4,4	0.31	0	6,6,6	0.11	0
2	SO4	B	364	-	4,4,4	0.38	0	6,6,6	0.15	0
2	SO4	C	364	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	C	365	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	W	364	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	X	364	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	Y	364	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	Y	365	-	4,4,4	0.35	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	364	-	-	0/0/0/0	0/0/0/0
2	SO4	B	364	-	-	0/0/0/0	0/0/0/0
2	SO4	C	364	-	-	0/0/0/0	0/0/0/0
2	SO4	C	365	-	-	0/0/0/0	0/0/0/0
2	SO4	W	364	-	-	0/0/0/0	0/0/0/0
2	SO4	X	364	-	-	0/0/0/0	0/0/0/0
2	SO4	Y	364	-	-	0/0/0/0	0/0/0/0
2	SO4	Y	365	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/365 (83%)	-0.33	0 100 100	15, 74, 94, 94	0
1	B	299/365 (81%)	-0.35	0 100 100	1, 54, 89, 94	0
1	C	329/365 (90%)	-0.37	1 (0%) 94 84	9, 65, 94, 94	0
1	D	297/365 (81%)	-0.35	1 (0%) 94 84	5, 69, 94, 94	0
1	W	296/365 (81%)	-0.36	0 100 100	7, 68, 94, 94	0
1	X	329/365 (90%)	-0.44	0 100 100	7, 68, 94, 94	0
1	Y	302/365 (82%)	-0.41	1 (0%) 94 84	1, 55, 89, 94	0
1	Z	301/365 (82%)	-0.33	2 (0%) 89 70	16, 74, 94, 94	0
All	All	2456/2920 (84%)	-0.37	5 (0%) 95 87	1, 66, 94, 94	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	PRO	3.7
1	Y	150	VAL	3.2
1	D	320	LYS	2.6
1	Z	314	GLY	2.1
1	Z	323	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	Y	364	5/5	0.93	0.12	-1.20	93,93,93,93	0
2	SO4	Y	365	5/5	0.91	0.17	-1.53	93,93,93,93	0
2	SO4	W	364	5/5	0.89	0.14	-1.55	93,93,93,93	0
2	SO4	B	364	5/5	0.80	0.13	-1.98	93,93,93,93	0
2	SO4	A	364	5/5	0.94	0.12	-2.06	93,93,93,93	0
2	SO4	X	364	5/5	0.88	0.13	-	93,93,93,93	0
2	SO4	C	364	5/5	0.88	0.12	-	93,93,93,93	0
2	SO4	C	365	5/5	0.88	0.15	-	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.